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A Python-Based Nuclear Data Visualization Package

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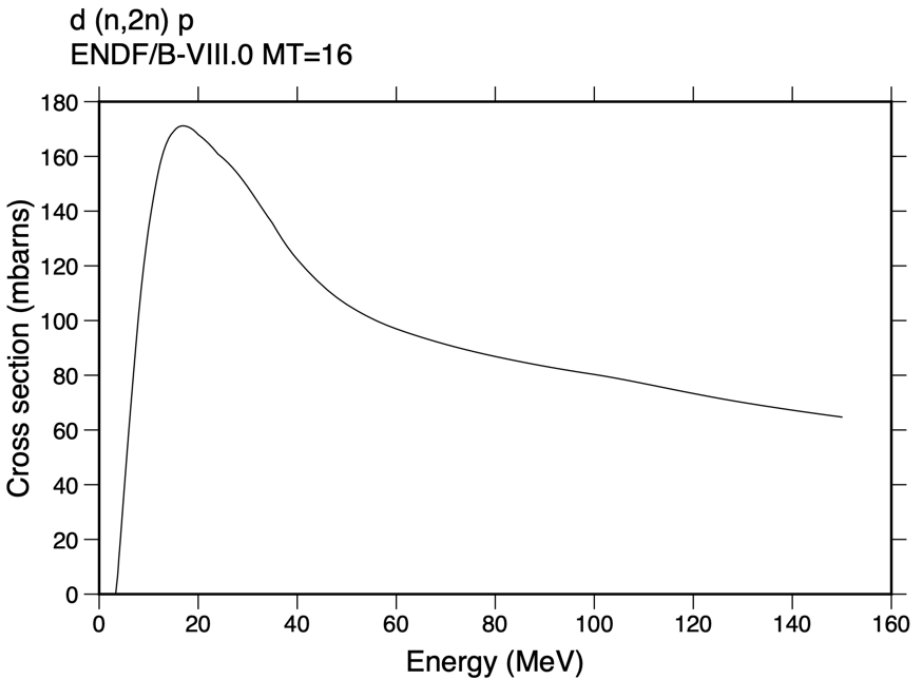
LA-UR-22-26977

Plotting in the NJOY Framework




```
plotr
  30 /
  / page
  1 0 1e-6 1e3 / new plot
  'd (n,2n) p' /
  'ENDF/B-VIII.0 MT=16' /
  1 /
  / x axis
  'Energy (MeV)' /
  / y axis
  'Cross section (mbarns)' /
  6 20 128 3 16 /
  /
  1 0 1e-6 1e3 / new plot
  't (n,2n) d' /
  'ENDF/B-VIII.0 MT=16' /
  1 /
  / x axis
  'Energy (MeV)' /
  / y axis
  'Cross section (mbarns)' /
  6 21 131 3 16 /
  /
  1 0 1e-6 1 / new plot
  'he3 (n,p) t' /
  'ENDF/B-VIII.0 MT=103' /
  4 /
  / x axis
  'Energy (MeV)' /
  / y axis
  /
  6 22 225 3 103 /
  /
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  'ENDF/B-VIII.0 MT=104' /
  1 /
  / x axis
  'Energy (MeV)' /
  / y axis
  'Cross section (mbarns)' /
  6 22 225 3 104 /
  /
  1 0 1e-6 1 / new plot
  't (p,n) he3' /
  'ENDF/B-VIII.0 MT=50' /
  1 /
  / x axis
  'Energy (MeV)' /
  / y axis
  'Cross section (barns)' /
  6 23 131 3 50 /
  /
  99 /

viewr
  30 31 /

stop
```
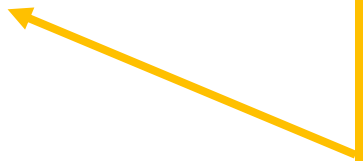

NJOY21 Project

- From-scratch effort to modernize NJOY
  - C++ with Python bindings
  - Open source (`github.com/njoy`)
  - Component-based approach
- Format components
  - ENDFtk
  - ACEtk
  - GNDStk



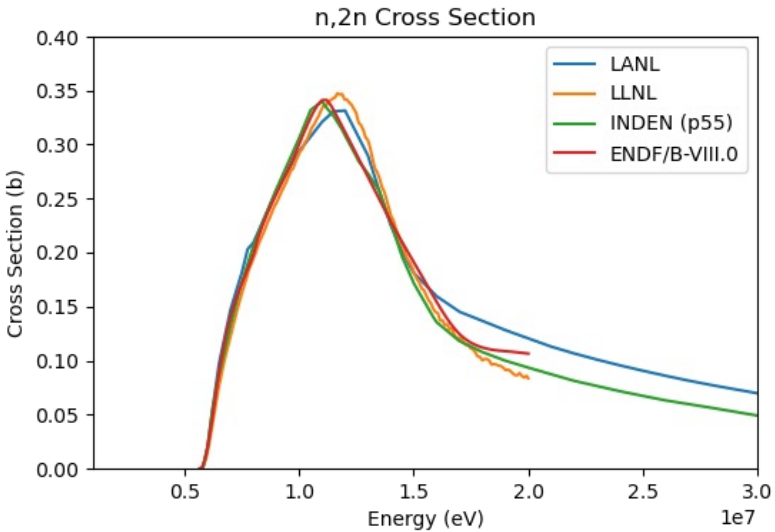
Opportunity for much more than end-to-end processing!

- Evaluator tools
- Perturbations
- User queries
- Data testing
- **Plotting**

Plotting in Python

Use Python-bound tools in conjunction with Matplotlib

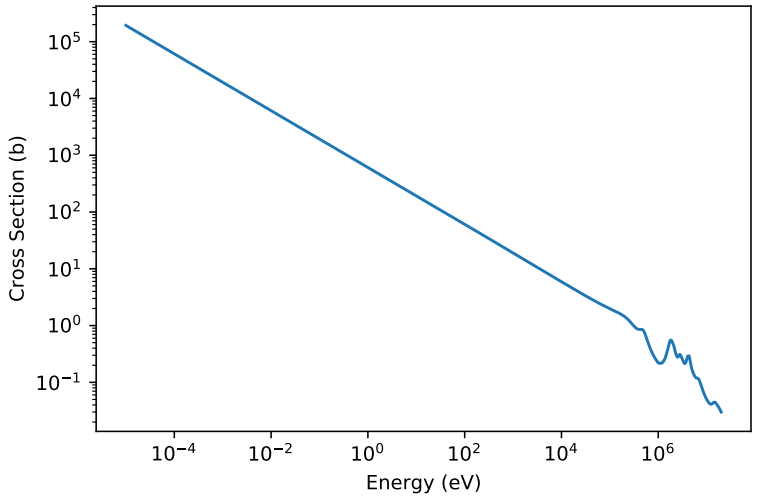
```
import ENDFtk
import matplotlib.pyplot as plt

def plot_cross_section(tape, mt, label):
    section = tape.MAT(9437).MF(3).MT(mt).parse()
    plt.plot(section.energies,
             section.cross_sections,
             label=label)
lanl_tape = ENDFtk.tree.Tape.from_file('lanl.endf')
plot_cross_section(lanl_tape, 16, 'LANL')
# ...

plt.xscale('log'); plt.xlim(1e4, 3e7); plt.ylim(0, 4)
plt.xlabel('Energy (eV)')
plt.ylabel('Cross Section (b)')
plt.title('n,2n Cross Section')
```

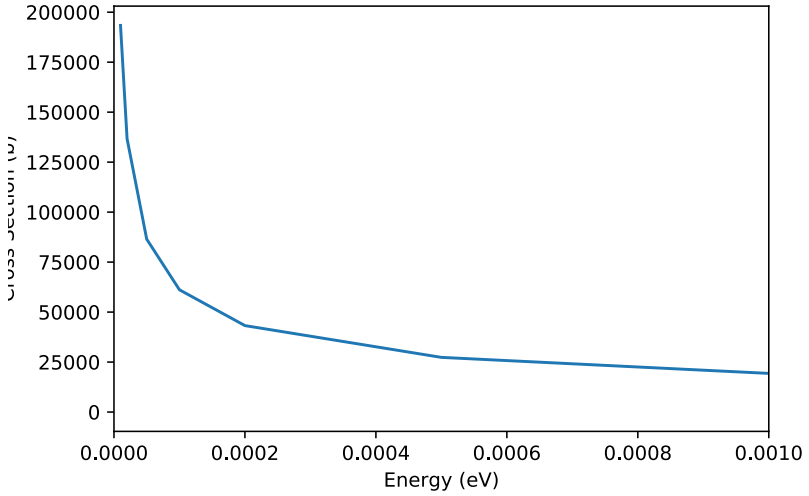


Needs Beyond Python Interface – 1/3

Linearization

Example: B-10 (n,alpha)





Needs Beyond Python Interface – 2/3

Interpretation

Example: Charged Particle Elastic Scattering

6.2. FORMATS

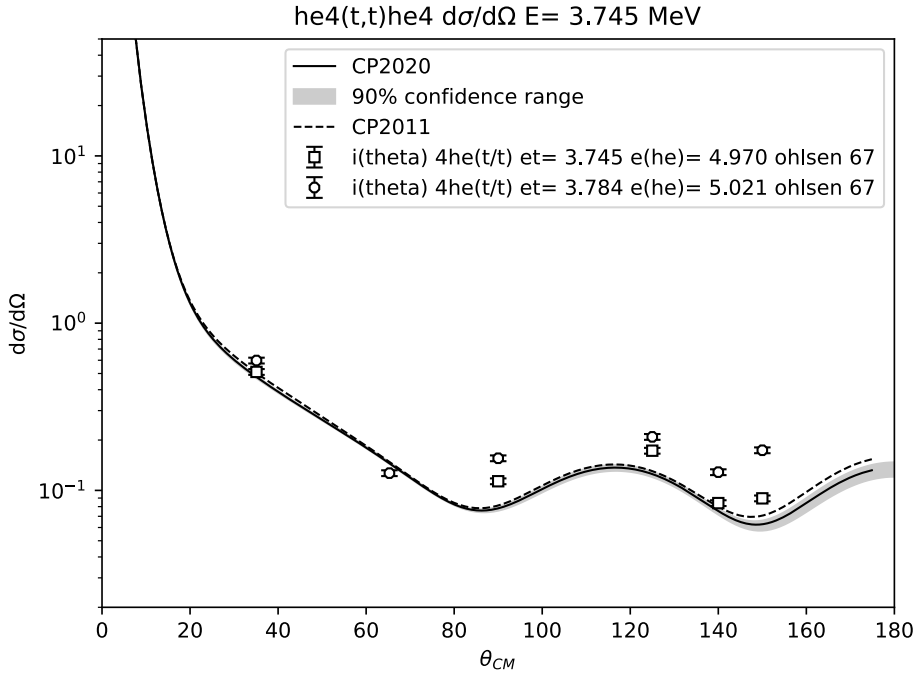
The cross sections can then be written:

$$\sigma_{cd}(\mu, E) = \frac{\eta^2}{k^2(1-\mu)^2} \tag{6.9}$$

$$\sigma_{ci}(\mu, E) = \frac{2\eta^2}{k^2(1-\mu^2)}\left[\frac{1+\mu^2}{1-\mu^2} + \frac{(-1)^{2s}}{2s+1}\cos\left(\eta \ln\frac{1+\mu}{1-\mu}\right)\right] \tag{6.10}$$

$$\text{where} \quad k = \frac{A}{1+A}\sqrt{\frac{2}{\hbar^2}\frac{u}{c^2}\, m_1 E} \times 10^{-14} \tag{6.11}$$

$$\eta = Z_1 Z_2 \sqrt{\frac{\alpha^2 u}{2}\frac{m_1}{E}} \tag{6.12}$$



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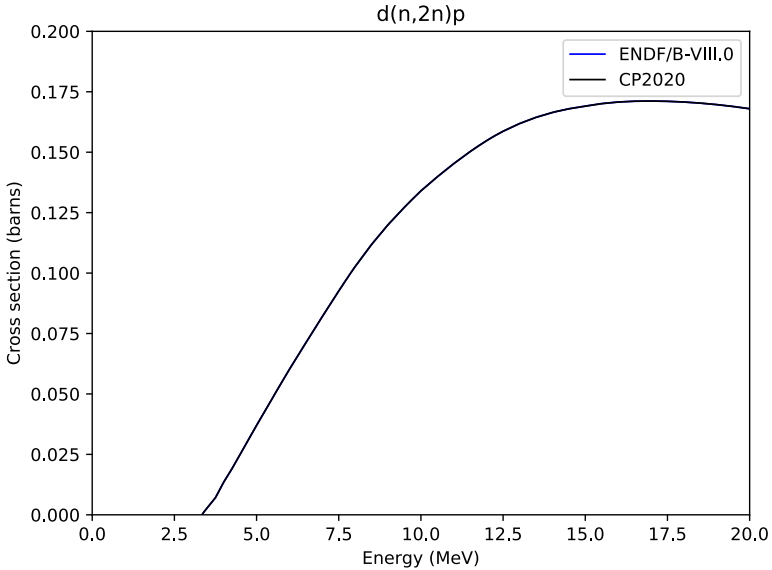
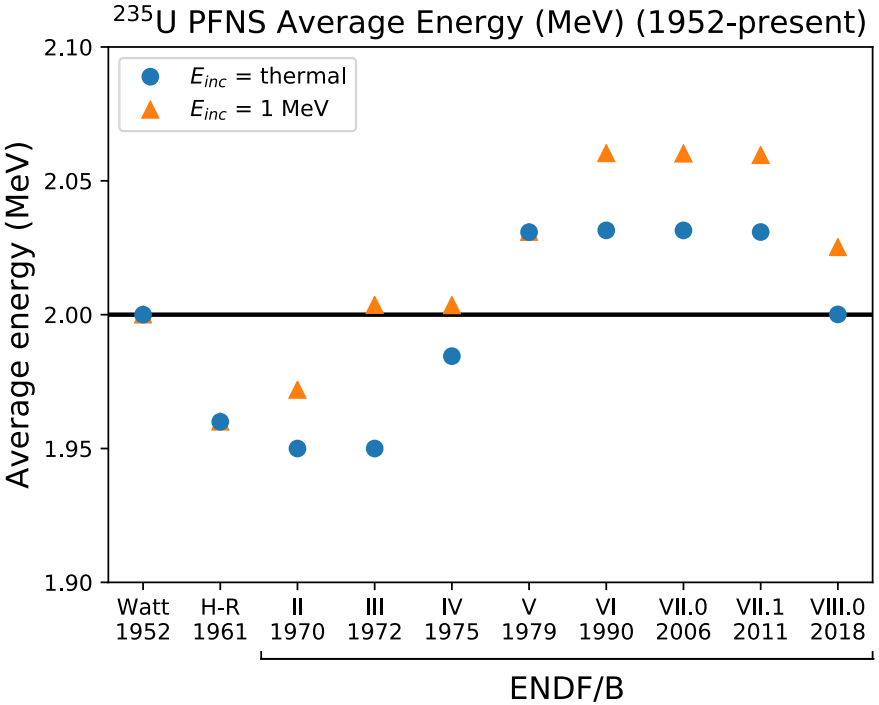
Needs Beyond Python Interface – 3/3

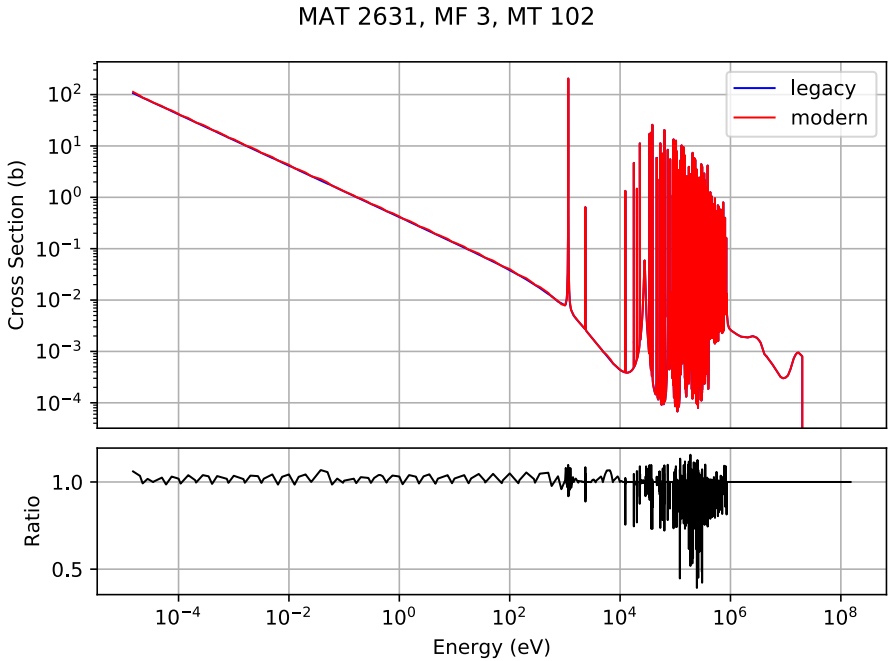
Interface



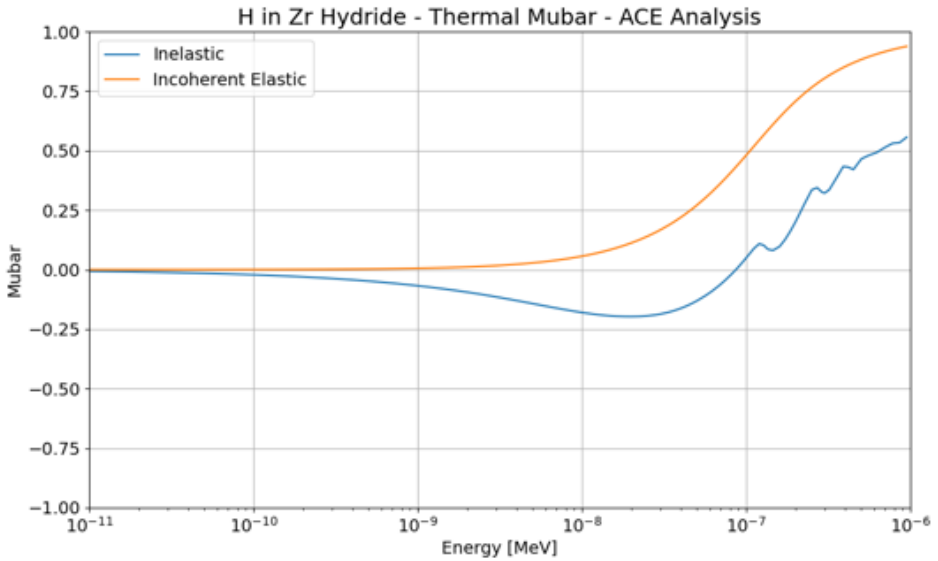

```
########################################
## PLOT 6
########################################

- curve:
    curvetype: ENDFCurve
    tape: 'endf8/neutrons/n-001_H_002.endf'
    section: [3, 16]
    label: 'ENDF/B-VIII.0'
    name: curve6-endf
    linecolor: b
    linewidth: 1
    units: MeV

- curve:
    curvetype: ENDFCurve
    tape: 'reconr/cp2020/n-001_H_002.endf'
    section: [3, 16]
    label: 'CP2020'
    name: curve6
    linecolor: k
    linewidth: 1
    units: MeV

- figure:
    figuretype: Figure
    title: 'd(n,2n)p'
    xlabel: 'Energy (MeV)'
    ylabel: 'Cross section (barns)'
    curves:
        - curve6-endf
        - curve6
    xlim: [0, 20]
    ylim: [0, .2]
    legend: True
    name: fig/tn06
```

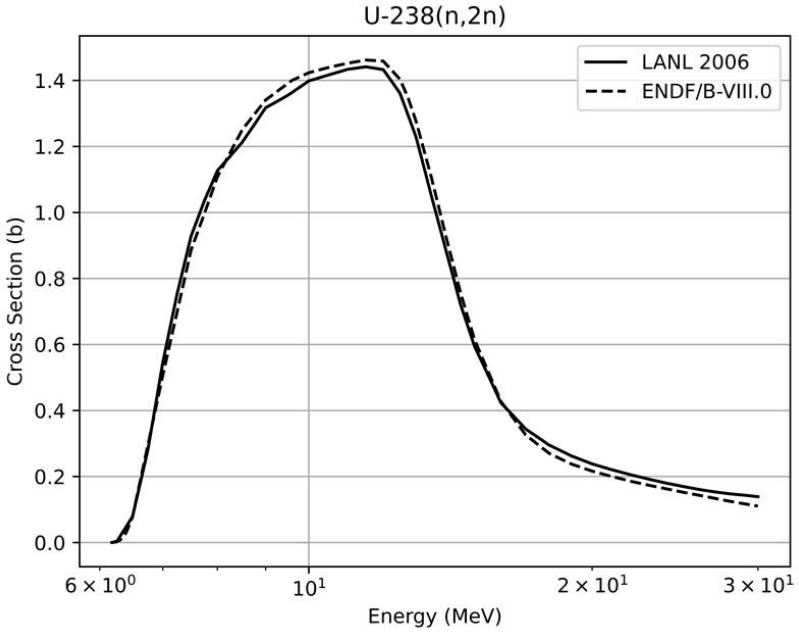
More Examples





Even More Examples (ACE)





Conclusions

- Open-source format interfaces are very useful for plotting
  - https://github.com/njoy/ENDFtk (develop)
  - https://github.com/njoy/ACEtk (fix/rounding)
- LANL is developing tools to improve experience and replace PLOTR
  - Linearization, interpretation, interface
  - Mixed formats support
- Contacts
  - ngibson@lanl.gov | njoy@lanl.gov | nucldata@lanl.gov

We're Hiring!

XCP-5 Nuclear Data Team is looking for postdocs and at least one early-to-mid-career scientist to work in areas such as:

- Pipeline modernization (automation, software, V&V, quality assurance)
- Data processing (developing NJOY and other tools, library generation)
- Uncertainty quantification (use of covariances, applications, ML methods)
- Evaluation support (bridging gap between science and application)

Job postings forthcoming. Contact ngibson@lanl.gov with questions.